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Electron paramagnetic resonance and optical spectroscopy of Yb3+ ions in SrF2 and BaF2; an analysis of distortions of the crystal lattice near Yb3+

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Abstract

SrF2 and BaF2 crystals, doped with the Yb3+ ions, have been investigated by electron paramagnetic resonance and optical spectroscopy. As-grown crystals of SrF2 and BaF2 show the two paramagnetic centres for the cubic (Tc) and trigonal (T4) symmetries of the Yb3+ ions. Empirical diagrams of the energy levels were established and the potentials of the crystal field were determined. Information was obtained on the SrF2 and BaF2 phonon spectra from the electron-vibrational structure of the optical spectra. The crystal field parameters were used to analyse the crystal lattice distortions in the vicinity of the impurity ion and the F- ion compensating for the excess positive charge in T4. Within the frames of a superposition model, it is shown that three F- ions from the nearest surrounding cube, located symmetrically with respect to the C3 axis from the side of the ion-compensator, approach the impurity ion and cling to the axis of the centre when forming T4. The F- ion located on the axis of the centre between the Yb3+ ion and ion-compensator, also approaches close to the impurity ion.

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